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Methods for High-order Multi-Scale and Stochastic Problems
Analysis, Algorithms, and Applications

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Final Report of AFOSR Grant F49550-12-1-0399
(The part of Chi-Wang Shu)

Methods for High-order Multi-Scale and Stochastic Problems Analysis, Algorithms, and Applications

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July 15, 2012 to July 14, 2016

1. Summary of research

We have performed research on the algorithm development, analysis, implementation and application for high order weighted essentially non-oscillatory (WENO) finite difference and finite volume schemes, discontinuous Galerkin (DG) finite element method, and related methods, for solving computational fluid dynamics (CFD) problems and other applications containing strong shock waves and complicated smooth region structures. The goal of this research is to help obtaining more robust, cost effective, and reliable numerical tools for computational fluid dynamics problems and other applications, that are of interest to AFOSR.

There are 17 publications in refereed journals, which have appeared or have been accepted for publications and have quoted partial support by this grant, see section 3.

In [1] (the numbers here and below refer to that of publications listed in section 3), we have explored an alternative formulation of finite difference WENO schemes with Lax-Wendroff time discretization for solving hyperbolic conservation laws. Even though this alternative formulation is more expensive than the standard formulation, it does have several advantages. The first advantage is that arbitrary monotone fluxes can be used in this framework, while the traditional practice of reconstructing flux functions can be applied only to smooth flux splitting. This allows us to choose monotone fluxes or approximate Riemann solvers with smaller numerical viscosity. The second advantage is that a narrower effective stencil is used compared with previous high order finite difference WENO schemes based on the reconstruction of flux functions, with a Lax-Wendroff time discretization. The third and major advantage is that free-stream-preserving high order finite difference WENO scheme can be designed

via this formulation, which keeps conservation, free-stream-preserving, and high order accuracy simultaneously. This advantage is fully explored with numerical experiments in [3]. The scheme in [3] has attracted a lot of attention from CFD applications, as it is a well-known difficult task to have conservation, free-stream-preserving, and high order accuracy fulfilled at the same time for high order nonlinear finite difference schemes.

In [2], a flux correction approach is used to design high order conservative finite difference and finite volume schemes which are positivity-preserving for density and pressure in Euler systems. Such methods are proved to maintain high order accuracy under mild assumptions. Computational results are provided in [2] to demonstrate the good performance of these schemes.

In [4], we study spectral collocation methods for functions which are analytic in the open interval but have singularities at end-points. Naive summation of the spectral partial sum leads to divergence near the end points and also poor convergence rate inside the interval. Previous techniques in post-preprocessing to overcome this difficulty do not apply because of the end-point singularities. We propose new analysis with suitable post-preprocessing, which leads to exponential accuracy in the maximum norm everywhere in the interval using only the information of point values at standard collocation points of such functions. The proof is constructive and provides guidance for practical implementation of the post-processor. Numerical experiments are given verifying the spectral convergence after post-processing. In [8], this technique and its analysis are generalized to Galerkin approximation and to the solution of linear PDEs. The techniques in [4] and [8] have already been used by other scientists to deal with interfaces in kinetic problems.

In [5], we design first order and higher order Lagrangian schemes for multi-material compressible flows, which are positivity-preserving for density and internal energy. Lagrangian schemes are particularly useful for solving multi-material compressible flows, as they keep the sharp interface between different materials during the evolution. However, stability for Lagrangian schemes is much more difficult to maintain than for Eulerian schemes. Especially for flows with general equations of state, even first order positivity-preserving schemes in multi-dimensions were not available before. We have constructed not only first order positivity-preserving Lagrangian schemes in multi-dimensions, but also higher order finite volume schemes with the same property. Numerical results demonstrate the good performance of these schemes for extreme flows, which lead to blowups of the scheme without the positivity-preserving techniques.

Recently, a class of schemes termed correction procedure via reconstruction (CPR) has been designed and used by aerospace engineers, who found the schemes performing well on both structured and unstructured meshes. However, for simulations with strong shocks, numerical oscillations may lead to nonlinear instability. In [6], we have adapted a simple WENO limiter which uses information only from immediate neighboring cells, originally designed for DG schemes, to the CPR schemes on un-

structured meshes. Numerical experiments indicate the good performance of this simple limiter which both keeps high order accuracy in smooth regions and controls spurious oscillations near shocks. Because the limiter uses information only from immediate neighboring cells, it does not destroy the original local data structure of the DG scheme and hence it maintains the major advantage of DG schemes in high parallel efficiency.

In [9], a well-designed adaptive mesh refinement (AMR) method based on high order finite difference WENO schemes is developed and applied to simulate three-dimensional detonation waves. Such simulations require large computational resources because of the high resolution requirement for the detailed detonation structure. The efficient parallel AMR-WENO method provides a good tool for these detonation simulations.

In [10], a predictive dynamic user-optimal traffic flow model in the continuum space with anisotropic condition is developed, which involves a coupled system of a forward-in-time conservation law for the traffic density and a backward-in-time Hamilton-Jacobi equation for the cost potential. This coupled system is very interesting mathematically, in terms of suitable assumptions for its well-posedness. More importantly, it provides a big challenge for its numerical simulation, as an iterative process would be needed (alternatively from forward in time with the Hamilton-Jacobi solution frozen, followed by backward in time with the conservation law solution frozen). We have explored such an iterative numerical method in [10] and tested it for this complex system.

The so-called inverse Lax-Wendroff procedure, which is a technique to obtain stable and accurate numerical boundary conditions when a cartesian mesh is used to solve a complex geometry problem (hence the grids are not aligned with the computational domain boundary), was proposed by the PI with his students a few years ago. This method has now found a wide usage in applications. In [11], we give a stability analysis, using both the GKS (Gustafsson, Kreiss and Sundström) theory and an eigenspectrum analysis, for this procedure applied to upwind-biased finite difference schemes for hyperbolic conservation laws. This study provides a theoretical guidance to determine the minimum number of terms needed in this procedure to guarantee stability, thus allowing us to design the most efficient yet guaranteed stable boundary treatments for such equations. In [17], similar stability analysis is performed for the central schemes approximating the diffusion equations. In [14], we have extended this technique to handle convection-diffusion equations including compressible Navier-Stokes equations, and have designed a procedure which works well across the convection-dominated to the diffusion-dominated regimes. This is a highly non-trivial task as boundary conditions play very different role for diffusion-dominated regimes and convection-dominated regimes, while our numerical procedure is expected to automatically adjust itself to yield stable and accurate algorithms across these two regimes. The inverse Lax-Wendroff procedure has already been used in several applications and is expected to play more important roles in the future.

Further development of this technique is now underway.

In [12], we have obtained a bound-preserving DG method for solving the relativistic hydrodynamics, which guarantees positive density and pressure and the upper bound of flow speed by the speed of light. This conservative scheme is then L^1 stable for all the conserved variables, which is rare for high order schemes solving hyperbolic systems.

A novel technique to use the idea of DG schemes to design a stable, conservative and high order accurate algorithm to solve hyperbolic conservation laws on an arbitrarily distributed point clouds is designed, analyzed and tested in [15]. By using the Voronoi technique and by introducing a grouping algorithm, we divide the computational domain into non-overlapping cells. Each cell is a polygon and contains a minimum number of the given points to ensure accuracy. We carefully select points in each cell during the grouping procedure, and hence are able to interpolate or fit the discrete initial values with piecewise polynomials. The DG framework allows us to design stable and accurate evolution algorithm on such polygonal cells, which have different number of sides for different cells and the cells may not be convex, causing significant difficulty for traditional finite element methods. Our algorithm provides good numerical results on the preliminary test cases in [15]. Further development of this technique is now underway.

In [16], a high order positivity-preserving DG method is designed for the radiative transfer equations, which involves a completely different strategy from previous techniques as the algorithm is a spatially marching type for steady states or implicit type for time-dependent problems. We have shown that the application of the simple scaling limiter, as is usually used in the explicit time marching case, would kill the order of accuracy beyond second order, and we have designed a rotational limiter which can be shown to maintain both the high order accuracy and positivity. The approach in [16] holds a good potential for leading to an efficient and robust high order DG solver for radiative transfer equations. Further development of this approach is now underway.

2. Broader impact

During the period of this AFOSR supported project, the co-PI, Professor Shu, taught several undergraduate and graduate level scientific computing courses covering related areas, and directed 10 Ph.D. students at Brown University (4 of them have already obtained their Ph.D. degrees, 2 in 2013, 1 in 2014 and 1 in 2015). Among these 10 Ph.D. students, 4 are women (women are underrepresented in mathematical sciences). The AFOSR grant greatly facilitated the offering of the courses and the training of these graduate students. It has also directly supported one graduate

student during this period.

3. Publications in refereed journals (appeared or accepted) which have quoted partial support by this grant

1. Y. Jiang, C.-W. Shu and M. Zhang, *An alternative formulation of finite difference weighted ENO schemes with Lax-Wendroff time discretization for conservation laws*, SIAM Journal on Scientific Computing, v35 (2013), pp.A1137-A1160.
2. X.Y. Hu, N.A. Adams and C.-W. Shu, *Positivity-preserving method for high-order conservative schemes solving compressible Euler equations*, Journal of Computational Physics, v242 (2013), pp.169-180.
3. Y. Jiang, C.-W. Shu and M. Zhang, *Free-stream preserving finite difference schemes on curvilinear meshes*, Methods and Applications of Analysis, v21 (2014), pp.1-30.
4. Z. Chen and C.-W. Shu, *Recovering exponential accuracy from collocation point values of smooth functions with end-point singularities*, Journal of Computational and Applied Mathematics, v265 (2014), pp.83-95.
5. J. Cheng and C.-W. Shu, *Positivity-preserving Lagrangian scheme for multi-material compressible flow*, Journal of Computational Physics, v257 (2014), pp.143-168.
6. J. Du, C.-W. Shu and M. Zhang, *A simple weighted essentially non-oscillatory limiter for the correction procedure via reconstruction (CPR) framework on unstructured meshes*, Applied Numerical Mathematics, v90 (2015), pp.146-167.
7. Y. Jiang, C.-W. Shu and M. Zhang, *High order finite difference WENO schemes with positivity-preserving limiter for correlated random walk with density-dependent turning rates*, Mathematical Models and Methods in Applied Sciences (M^3AS), v25 (2015), pp.1553-1588.
8. Z. Chen and C.-W. Shu, *Recovering exponential accuracy in Fourier spectral methods involving piecewise smooth functions with unbounded derivative singularities*, Journal of Scientific Computing, v65 (2015), pp.1145-1165.
9. C. Wang, X. Dong and C.-W. Shu, *Parallel adaptive mesh refinement method based on WENO finite difference scheme for the simulation of multi-dimensional detonation*, Journal of Computational Physics, v298 (2015), pp.161-175.

10. J. Du, S.C. Wong, C.-W. Shu and M. Zhang, *Reformulating the Hoogendoorn-Bovy predictive dynamic user-optimal model in continuum space with anisotropic condition*, Transportation Research Part B, v79 (2015), pp.189-217.
11. T. Li, C.-W. Shu and M. Zhang, *Stability analysis of the inverse Lax-Wendroff boundary treatment for high order upwind-biased finite difference schemes*, Journal of Computational and Applied Mathematics, v299 (2016), pp.140-158.
12. T. Qin, C.-W. Shu and Y. Yang, *Bound-preserving discontinuous Galerkin methods for relativistic hydrodynamics*, Journal of Computational Physics, v315 (2016), pp.323-347.
13. C.-W. Shu, *High order WENO and DG methods for time-dependent convection-dominated PDEs: a brief survey of several recent developments*, Journal of Computational Physics, v316 (2016), pp.598-613.
14. J. Lu, J. Fang, S. Tan, C.-W. Shu and M. Zhang, *Inverse Lax-Wendroff procedure for numerical boundary conditions of convection-diffusion equations*, Journal of Computational Physics, v317 (2016), pp.276-300.
15. J. Du and C.-W. Shu, *A high order stable conservative method for solving hyperbolic conservation laws on arbitrarily distributed point clouds*, SIAM Journal on Scientific Computing, to appear.
16. D. Yuan, J. Cheng and C.-W. Shu, *High order positivity-preserving discontinuous Galerkin methods for radiative transfer equations*, SIAM Journal on Scientific Computing, v38 (2016), pp.A2987-A3019.
17. T. Li, C.-W. Shu and M. Zhang, *Stability analysis of the inverse Lax-Wendroff boundary treatment for high order central difference schemes for diffusion equations*, Journal of Scientific Computing, to appear.

**FINAL REPORT ON AFOSR FA9550-12-1-0399
OPTIMAL CONFORMING HIGH ORDER FINITE
ELEMENT COMPUTATION VIA BERNSTEIN-BÉZIER
POLYNOMIALS**

MARK AINSWORTH

1. BACKGROUND

The classical finite element method, based on low order piecewise polynomial approximation using Lagrange shape functions in conjunction with mesh refinement, offers geometric flexibility but suffers from relatively poor resolution. The spectral method, on the other hand, achieves high resolution by employing a fixed mesh (often a single element) in conjunction with very high degree polynomial approximation, but suffers from a lack of geometric flexibility compared with the finite element method. The spectral/*hp*-version finite element method aims to combine the advantages of each approach by using high degree piecewise polynomials in a finite element setting.

High order finite element methods have been analysed extensively for a wide variety of applications and are known to be capable of producing exponential rates of convergence, even for challenging problems with singularities, sharp boundary layers, and high frequency oscillations. High order polynomial approximations are commonplace in many areas of scientific computing including computer graphics, computer aided-geometric design, and spectral methods for PDEs. It is commonplace to see the spectral method used with approximation orders in the 100s or 1000s.

Yet, despite theory giving the nod to the use of very high order finite element methods, the range of polynomial degree used in practical finite element computations is rarely larger than *eighth* order! Possible explanations for the use of comparatively modest polynomial orders include issues of efficiency, implementation, and stability. Moreover, existing implementations of high order finite elements tend to be memory hungry, often relying on the use of precomputed arrays and look-up tables, a feature that does not augur well for the future given the nature of emerging computer hardware systems. Whatever the underlying reasons, it is clear that the rather modest polynomial degrees seen in high order finite element analysis are due to practical considerations rather than any theoretical barriers.

The proposed programme of research is directed towards tackling these issues.

Date: October 9, 2016.

2. ALGORITHMS FOR BERNSTEIN-BÉZIER FINITE ELEMENTS OF HIGH, NON-UNIFORM ORDER IN ANY DIMENSION

The archetypal *pyramid algorithm* is the de Casteljau algorithm; a standard tool for the evaluation of Bézier curves and surfaces, and polynomials expressed in Bernstein-Bézier form in general. The algorithm enjoys widespread usage, despite being sub-optimal, thanks to the ease with which it can be implemented, its underlying stability properties and short, simple recursive nature with minimal memory overhead. In essence, the de Casteljau algorithm replaces a single high order polynomial by a recursive sequence of self-similar affine combinations. Pyramid algorithms are ubiquitous in the computer aided geometric design community for computations using high order curves and surfaces. Pyramid algorithms have received no attention whatsoever from the high (or low) order finite element community. In the article [1] we develop and analyse pyramid algorithms for the efficient handling of all of the basic finite element building blocks, including the assembly of the element load vectors and element stiffness matrices.

Hierarchic bases have been prevalent throughout the high order finite element literature from the very outset. The first step towards developing pyramid algorithms for high order finite elements is to dispense with hierarchic bases in favour of the non-hierarchic, Bernstein-Bézier (BB-) basis. Some practitioners may balk at this prospect, pointing to the freedom hierarchic bases bring to allow varying local approximation order of the elements. However, we shall see that pyramid algorithms bring the same flexibility to the (non-hierarchic) BB-basis at *no additional complexity*, but, in addition, with the usual advantages associated with pyramid algorithms. Bernstein-Bézier bases have recently been shown to offer some advantages for uniform order finite element approximation.

We begin by generalising the Bernstein Decomposition for uniform approximation order, to the variable order setting. A non-uniform order Bernstein-Bézier basis emerges for which the enforcement of conforming between elements of differing local orders is a natural consequence of the structure of the non-uniform order Bernstein Decomposition.

A new, non-uniform order, variant of the de Casteljau algorithm is developed (expressed as a pyramid algorithm) that retains the favourable features of the original algorithm. The new variant is applicable to the variable polynomial order case but incurs no additional complexity compared with the original algorithm. The classical degree raising algorithm is given a similar treatment giving a new, non-uniform order, degree raising pyramid algorithm. Yet more interestingly, the *dual pyramid* of our non-uniform order degree raising algorithm gives a pyramid algorithm for the assembly of the non-uniform order element load vector. The complexity of the algorithm is the same as that of the most efficient hierarchic bases currently in use.

An algorithm for the construction of the element matrices in optimal complexity for uniform order approximation on a simplicial elements was

developed only recently [2]. The efficiency of that algorithm uses the underlying uniformity of the polynomial order across the element in an essential way. There is no existing algorithm that constructs the non-uniform order element matrices in optimal complexity. In the final part of this work, we extend the algorithm of [2] to the non-uniform order case. Moreover, we show that the resulting algorithm achieves the optimal complexity.

In summary, the article [1] provides the methodology that enables the efficient use of a completely general distribution of polynomial degrees without any restriction in changes between adjacent cells on simplicial partitions in any number of spatial dimensions.

3. BERNSTEIN-BÉZIER FEM ON TET-HEX-PYRAMIDAL MESHES

In theory at least, finite element approximation on a three dimensional domain differs little from approximation over planar domains. However, the reality is that one is beset by various niggling issues not least of which is the choice of a partitioning for the domain. On the one hand, hexahedral elements are often preferred for reasons of efficiency stemming from the tensor-product nature of the elements and the underlying approximation space, but the practical issues of meshing a complicated three dimensional geometry using only hexahedra should not be underestimated. On the other hand, while there are many efficient algorithms available for meshing using tetrahedral elements, the numbers of degrees of freedom in the resulting finite element space generally significantly exceed what would be needed should a hexahedral partitioning be available, without a commensurate improvement in accuracy.

An obvious solution would seem to consist of using a partition comprised of a mix of both tetrahedra and hexahedra with hexahedra used as much as possible, with the tetrahedra used to mesh the remaining more complicated geometrical features. This would be fine were it not for the fact that tetrahedra and hexahedra fail to tessellate. Again, a possible solution readily suggests itself whereby pyramidal elements are used as a means of interfacing between the tetrahedra with the hexahedra.

The question then becomes one of how to define shape functions on the pyramids in such a way as to obtain globally C^0 (conformal) test functions. The problem now is that it is impossible to do this using polynomial basis functions. Various approaches have been taken to solving this problem. The upshot is that non-polynomial basis functions are required which, in turn, gives rise to further difficulties associated with numerical integration and the analysis.

At this point, one might be left with a growing feeling that hybrid partitions may be more trouble than they are worth. Nevertheless, the current work presents a fresh approach to dealing with the pyramidal transition elements which: avoids the need for non-polynomial functions in favour of using piecewise polynomials, and as such is entirely in keeping with the spirit of

the finite element method; neatly side steps technical questions associated with the error of the quadrature and approximation power of the spaces; and, opens up the possibility for adopting fast (optimal complexity) algorithms developed in our previous work [2] for the system matrix assembly and matrix-free implementations.

In the article [4] we characterise the hybrid partitions of interest. While this might seem to be straightforward, in practice, it is of considerable interest to allow partitions in which the faces of the hexahedra are allowed to be bilinear quadrilaterals. In turn, this means that one is obliged to consider pyramids whose quadrilateral face is bilinear, which is generally disallowed in existing work on pyramidal elements. We therefore devote attention to carefully defining pyramidal elements of this type and characterizing conditions under which associated maps to the reference element are invertible. The bilinear face of the pyramid means that the splitting of the pyramid into interface tetrahedra is not straightforward. We discuss the appropriate way to split pyramids into a pair of interface tetrahedra which, of necessity, must be curvilinear. We introduce the approximation space to be used in the finite element method, and give a concrete construction of the shape functions associated with each of our elements. We discuss domain points and minimal determining sets, and we use these concepts to find a formula for the dimension of our spline space and to construct a locally supported basis for it. Finally, we collect some useful computational algorithms for dealing with Bernstein basis polynomials from our previous work, which are then used in to develop algorithms for efficiently computing all of the various quantities needed for a finite element analysis and evaluation of the resulting approximation. Finally, the approximation power of our spline space is proved.

4. BERNSTEIN-BÉZIER BASIS FOR ARBITRARY ORDER MIXED FEM

Bernstein polynomials play an important role in CAGD and possess a number of interesting properties that have led to their widespread usage in a range of applications. Historically, hierarchic polynomial bases have been used virtually exclusively for high order finite element approximation. However, the Bernstein basis is more natural with the degrees of freedom being more akin to the nodal degrees of freedom described in most finite element textbooks. More importantly, it was recently shown that using a Bernstein basis for the standard H^1 -conforming finite element spaces enables the mass and stiffness matrices to be constructed in optimal complexity [2] in terms of the polynomial degree. The algorithms take advantage of properties of Bernstein polynomials and the *sum-factorisation* approach that provides the cornerstone of the spectral method.

In [3] we extend the ideas of [2] to the case of conforming finite element approximation of the space $\mathbf{H}(\text{div})$ on triangulations. We seek a basis that gives a clear separation between what are sometimes termed the *curls* of

the Bernstein polynomial basis for the H^1 space, and the non-curls that characterize the specific $\mathbf{H}(\text{div})$ finite element space (Raviart-Thomas in our case). The resulting basis has two distinct components reflecting this separation with the basis functions in each component having a natural identification with a domain point, or node, on the reference element in contrast with the hierarchic finite element bases developed hitherto. More importantly, it is shown that the basis retains the favourable properties of the Bernstein basis that were used in [2] to develop efficient computational procedures for the application of the elements.

5. SOLUTION OF BERNSTEIN-VANDERMONDE SYSTEMS

The Bernstein-Bézier (BB) representation of a polynomial $p \in \mathbb{P}^n([0, 1])$ takes the form $p = \sum_{k=0}^n c_k B_k^n$ in which the coefficients $\{c_k\}$ are referred to as *control points*. However, while the polynomial p satisfies $p(0) = c_0$ and $p(1) = c_n$, this property does not hold at the remaining control points. On the one hand, this property does not hinder the typical workflow of a CAGD engineer whereby the locations of $\{c_k\}$ are adjusted until a curve of the desired shape is obtained. In effect, the control points are used to *define* the curve directly. On the other hand, the typical usage of polynomials in scientific computing is rather different in that one generally wishes to *fit* a polynomial to a given function. For example, in applying the finite element method to approximate the solution of a partial differential equation, one might have boundary or initial data and require to choose an appropriate (piecewise) polynomial approximation of the data. The approximation is often chosen to be an interpolant, leading to what we shall term the Bernstein-Bézier interpolation problem, which consists of computing the control points $\{c_k\}_{k=0}^n$ such that the associated Bernstein-Bézier polynomial interpolates the data:

$$p(x_j) = \sum_{k=0}^n c_k B_k^n(x_j) = f_j, \quad j = 0, \dots, n. \quad (1)$$

Conditions (1) may be expressed as a system of linear equations involving the *Bernstein-Vandermonde* matrix. If the monomial basis were to be used, then the standard Vandermonde matrix would emerge. The highly ill-conditioned nature of the Vandermonde matrix is well-documented. Notwithstanding, the inversion of the Vandermonde matrix to compute the Lagrangian interpolant is in some ways preferable to more direct methods.

The Bernstein-Vandermonde matrix is likewise found to be highly ill-conditioned, though to a lesser extent than the Vandermonde matrix, suggesting that its inversion may not be the wisest approach. Nevertheless, *structure* of the matrix arising from the *total positivity* of the Bernstein basis means that using Neville elimination to solve the system obviates some of the issues due to ill-conditioning. Marco and Martínez exploit this fact

and derive an algorithm for the inversion of the matrix that has $\mathcal{O}(n^2)$ complexity—the same as multiplying by the inverse of the matrix.

Remarkable though the Marco-Martínez algorithm may be, it does have its drawbacks:

- the derivation of the algorithm is highly technical involving non-trivial identities for the minors of Bernstein-Vandermonde matrices;
- the interplay between the ideas of total positivity, bidiagonal factorisation and Neville elimination are not part of the standard armoury of many non-specialists;
- the algorithm seems to be firmly rooted to the solution of the Bernstein interpolation problem in the univariate case when simplices are considered (indeed, total positivity is essentially a univariate concept).

In [5] we address these issues. Specifically, we present an alternative algorithm for the inversion of the univariate Bernstein-Vandermonde system that has:

- the same complexity as the Marco-Martínez algorithm and whose stability does not seem to be in any way inferior;
- a simple derivation that could be taught to undergraduates familiar with only the basic theory of Lagrange interpolation (at least in the univariate case);
- a natural generalisation to the multivariate case on simplices (essential for applications such as finite element analysis in two and three dimensions).

More specifically, we derive the new algorithm in the univariate case using only elementary facts about univariate interpolation and basic properties of Bernstein polynomials, and present a straightforward extension of the univariate algorithm to the multivariate tensor product case. We tackle the much harder task of solving the Bernstein interpolation problem on simplices in higher dimensions in which even the existence of the Lagrangian interpolant is less obvious. Using the standard hypothesis under which the Lagrange interpolant exists, we develop an algorithm for the solution of the multivariate Bernstein interpolation problem on simplices in two dimensions, and indicate how it may be extended to arbitrary dimensions. The ideas used are, modulo technical issues, essentially the same to those used in Section 2 to handle the univariate case. We give numerical examples illustrating the behaviour and stability of the resulting algorithms.

The algorithms developed in the present work form a key step towards a more widespread use of Bernstein-Bézier techniques in scientific computing in general, and in finite element analysis in particular by enabling the use of non-homogeneous initial and boundary data. More generally, the problem of how to solve Bernstein-Vandermonde systems on simplices in arbitrary dimension is addressed.

6. PERSONNEL INVOLVED IN RESEARCH SUPPORTED BY THE AWARD

- Mark Ainsworth, Professor, Brown University.
- Christian Glusa, Graduate Student, Brown University.
- Manuel Sanchez-Urbe, Graduate Student, Brown University.
- Oleg Davydov, Research Visitor, Universität Giessen, Germany.

7

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1 Stability and Numerics for Weakly Interacting Particle Systems

1.1 Problem formulation and issues

Many physical and engineering systems can be modeled as a large collection of stochastically evolving agents or particles, whose dynamics are weakly coupled by an interaction that depends only on the distribution of the particles. Simulations of these systems has shown that the dynamics of these systems exhibit interesting and complex behavior. The number of particles is typically large, and there are no general purpose tools for analyzing such systems that are both accurate and computationally feasible. Of particular interest are the long-term stability and metastability properties of these systems.

This part of the research project was concerned with the development of general mathematical methods, both analytical and numerical, to study the long-time behavior, metastability properties and control of such stochastic systems. In many cases, the N particles are exchangeable and the relevant quantities are captured by the empirical distribution of the N -particle system. We studied two classes of problems, one when the state of each particle is discrete, taking a finite number of values, and when the state of each particle is a continuum, for example, the whole real line. As described below, the methods used in each of the two cases are somewhat different.

1.2 Results and Key Findings: The Finite-Dimensional Case

1.2.1 Accelerated Monte Carlo and large and moderate deviations

One focus was on the use of large deviation methods for accelerated Monte Carlo schemes. Specifically, we used large deviation theory for purposes of design and analysis, and when existing theory is not adequate, it was developed in the form suited to such applications. The large deviation theory for various process models was developed in [BCD13, DJ15] and [BDG16]. It is known that when using any of the standard methods that reduce variance and thereby improve efficiency one needs some information on the conditional distributions of the associated process model. Also, in the setting of rare events the use of accelerated Monte Carlo is essential, since the relative variance (i.e., the variance of the sample to the size of the probability being estimated) scales inversely to the size of the probability.

The papers [DJ15] and [BDG16] prove what are called moderate deviation principles (or moderate deviation approximations) for fairly complicated process models. A moderate deviation principle gives information that is not as far out in the tails of the distribution as in the case of large deviation, and hence can be used to study events that are rare but not extremely small. When using a moderate deviation approximation one is typically interested in accelerated methods because the expense associated with generating even a single sample can be high.

As an example of how the results of [BDG16] could be used consider the problem of assessing the probability of exceeding an allowed pollution level in the context of groundwater contamination. Pollutants are modeled as entering a waterway according to a spatially distributed Poisson input, after which they diffuse throughout the waterway. The problem of interest might be a rare event, such as exceeding a regulatory threshold for chlorinated hydrocarbons, or a less rare event, such as higher-than-normal levels of plant nutrients, leading to algae bloom and fish kill. Each sample thus requires the solution of a 2 or 3 dimensional partial differential equation.

The process models covered in [DJ15] are more directly relevant to the project’s overall goals, and include weakly interacting many particle models with a finite dimensional empirical measure (e.g., weakly interacting finite state Markov chains). Here again one is especially concerned with variance reduction due to the fact that simulating even a single sample is costly when the number of particles is large.

For both the large deviation and moderate deviation approaches the construction of accelerated Monte Carlo schemes are based on subsolutions to a nonlinear partial differential equation (PDE) associated with the rate function of the process. It is the rate function which gives approximations to conditional distributions of the process. In general one expects the moderate deviations rate function to involve a linear approximation of the dynamics and a quadratic approximation of the costs found in the large deviations rate function, centered around the law of large numbers limit. This corresponds to a “local Gaussian” approximation, and the PDEs involved are those associated with the famous “linear-quadratic-regulator,” whose solution can be constructed in terms of the solution to an appropriate Riccati equation.

In [DJ16] the moderate deviation results of [DJ15] are applied to the design of efficient importance sampling schemes. We present various implementations, and include numerical results to contrast their performances, including weakly interacting particle models. Also included is a discussion under what circumstances a particular scaling (large or moderate) is most appropriate. Owing to the fact that the linear-quadratic-regulator has (up

to the solution of a Riccati equation) has an explicit solution, the design of optimal and nearly optimal schemes can be done in great generality.

1.2.2 Robustness and model error in the context of rare events

There is little known regarding the robustness of large deviation estimates with regard to modeling errors. This is the problem treated in [ACD15], which builds on ideas first developed in [CD13]. In [ACD15], we extend the duality between exponential integrals and relative entropy to a variational formula for exponential integrals involving the Rényi divergence. This formula characterizes the dependence of risk-sensitive functionals to perturbations in the underlying distribution. It also shows that perturbations of related quantities determined by tail behavior, such as probabilities of rare events, can be bounded in terms of the Rényi divergence. The characterization gives rise to tight upper and lower bounds that are meaningful for all values of a large deviation scaling parameter, allowing one to quantify in explicit terms the robustness of risk-sensitive costs. As applications we consider problems of uncertainty quantification when aspects of the model are not fully known, as well their use in bounding tail properties of an intractable model in terms of a tractable one.

1.2.3 Cooperative control of many particle systems

In [DRV16] we study many particle exit time stochastic control problems with risk-sensitive cost. Each particle takes values in a finite set \mathcal{X} , and by controlling the rates of each individual the aim is to keep the system away from a “ruin” set \mathcal{K} for as long as possible and with the least cost. We prove, under suitable assumptions, that for every finite number n of particles the control problem is equivalent to one with an ordinary (additive) cost. Moreover, when $\mathcal{K} \subset \mathcal{X}^n$ can be identified with a subset of the simplex of probability measures $\mathcal{P}(\mathcal{X})$ (in the sense that for every permutation $\sigma \in \mathbb{S}_n$ we have $\sigma\mathcal{K} = \mathcal{K}$), then we can replace the original problem by one on $\mathcal{P}^n(\mathcal{X}) = \mathcal{P}(\mathcal{X}) \cap \frac{1}{n}\mathbb{Z}^d$, getting in this way a control problem whose state is the empirical measure on the states of the individual particles.

We start with a collection of independent particles/agents with each evolving according to the transition rates γ . This is the “preferred” or “nominal” dynamic, and is what would occur if no “outside influence” or other form of control acts on the particles. If a controller should wish to change this behavior, then it must expect to pay a cost to do so. We model the situation where limited information on the system state, and in

particular information relating only to the empirical measure of the states of all particles, is used to produce a desired behavior of the group of particles, which again will be characterized in terms of their empirical measure (how the collective “loads” the system).

The paper presents three results. The first is that, under certain conditions, for each n the risk-sensitive control problem is equivalent to an ordinary control problem rather than a *stochastic game*, as one might expect. We also show under appropriate conditions that both the risk sensitive and the ordinary control problems are equivalent to mean field control problems. The last contribution is convergence of a suitably normalized value functions for the n particle system to the value function of a deterministic control problem.

1.3 Results and Key Findings: The Infinite-dimensional Case

1.3.1 Network models

Large-scale stochastic networks arise in a variety of of real world applications, ranging from telecommunications, service systems and computer networks to health care services and biological systems. Such networks are typically too complex and not amenable to exact analysis. However it is often possible to provide insight into network performance, in both the transient and equilibrium regimes, through tractable approximations. Finite-dimensional Markov processes have been used extensively in the literature to describe the scaling limits of stochastic networks under simplifying assumptions such as exponential service distributions. However, statistical analysis has shown that the service distribution is typically non-exponential.

In the works [A15] and [A16a], the authors study the classical model of an N -server queue with cumulative renewal arrivals and jobs with i.i.d. service distribution served in a First-Come-First-Serve (FCFS) manner. It was shown in earlier work of Kaspi and Ramanan (2011) that such a system can be viewed as a weakly interacting particle system in which each particle corresponds to a server, and the state of the system is the amount of time that the server has spent serving the job it currently has in system (or, is in an idle state, if it is not serving any job). Since the servers are exchangeable, the dynamics is captured by the empirical measure of the state of the servers. Kaspi and Ramanan (2011) established a certain functional laws of numbers limit for this measure-valued system, and subsequently, in 2013, established a functional central limit theorem. Both of these limit theorems captured the mean behavior and fluctuations around the mean behavior on finite time

intervals. A major open problem posed by Halfin and Whitt in 1981, was to obtain an approximation for the diffusion-scaled steady state distribution of this network. A key challenge was that, due to the infinite-dimensional of the state-space, classical Lyapunov function and positive Harris recurrence techniques are not applicable. In [A15] and [A16a] we introduce new methods that rely on the framework of asymptotic coupling recently introduced by Hairer, Mattingly and Scheutzow and others to show (for a large class of service distributions) convergence of the diffusion scaled N -server queue lengths to a limit, that can be characterized as the unique stationary distribution of an infinite-dimensional Markov process.

The methods introduced in [A15] and [A16a], in particular certain asymptotic coupling constructions, are more broadly applicable for study of a much broader class of networks, and provide a major first step in developing analytical characterizations and numerical methods for estimating the limit steady-state distribution.

The work in [A16b] studies a more complicated many-server model with randomized load balancing, in which each server has its own dedicated queue. This system can once again be represented by a weakly interacting particle system, whose dynamics is captured by interacting measure-valued processes. This randomized load balancing network had earlier only been analyzed in the case of exponential service distributions independently by Mitzenmacher and by Dobrushin, Karpelevich and Vvydenskaya. Our work provides a framework for analyzing such models in the presence of general service distributions. In particular, in [A16b] we show that, as the number of servers N goes to infinity, the measure-valued process that captures the dynamics of the load balancing network, converges to a hydrodynamic limit. This allows one to study the impact of the service distribution on the performance. Our general framework is also useful for the study of a much broader class of many-server load balancing networks.

1.3.2 Particles with Singular Interaction

There is a substantial interest in interacting particle systems in which each particle takes values in the reals, and the n -particle configurations follow a Gibbs distribution, which is parameterized by a quantity (often referred to as the inverse temperature β_n) and an energy functional that is the sum of a (possibly singular) interaction W and a confining potential V . Such processes model a variety of systems of interest including interacting Brownian particles, eigenvalues of random matrices, and arise in the study of sampling and simulated annealing. In particular, it is of interest to study probabilities

of rare events in such systems, when the number of particles is large. In [DLR15] we establish large deviation principles (LDPs) for empirical measures associated with a sequence of Gibbs distributions of n -particle configurations associated with the parameter β_n , both with speeds $\beta_n/n \rightarrow \infty$,

While the case when the interaction W is bounded is well-studied, in the applications mentioned above, W may blow up along the diagonal. In [DLR15], in which case the rate function is expressed in terms of a functional involving the potentials, and with the speed $\beta_n = n$, when the rate function contains an additional entropic term. Using the weak convergence methods first introduced by Dupuis and Ellis we establish large deviation principles not only with respect to the weak topology, but also with respect to stronger, Wasserstein-type topologies, which allows one to also understand the behavior of unbounded continuous functionals of the empirical measure of the particles, such as moments, which are of interest in applications. Our work provides a common framework for the analysis of LDPs with all speeds, and includes cases not covered due to technical reasons in previous work of Ben Arous et. al (1998) and Chafai (2014).

1.3.3 Sensitivities of Constrained Processes

Reflected stochastic processes that are constrained to lie in the closure of a convex polyhedral domain arise in many contexts, including as diffusion approximations of stochastic networks, in the study of interacting diffusions and limits of interacting particle systems, in chemical and biochemical reaction networks and in mathematical finance. The analysis of processes with state constraints is challenging due to the fact that the nature of the dynamics often changes abruptly at the boundary of the domain, and is further complicated when the boundary is not smooth. Given that in many models, there is uncertainty in the parameters that define the system, a key question of interest is the dependence of the reflected process (in particular, expectations of functionals of the process) on various parameters that define it.

The sensitivity of the stochastic process to perturbations in the initial condition and other parameters that define the process, is a classical topic in stochastic analysis. For example, there is a substantial body of work that studies these questions for (unconstrained) diffusions in Euclidean space, with contributions from Elworthy (1978), Bismut (1981), Ikeda and Watanabe (1981), Kunita (1981), Metivier (1982) and others. In contrast, there are relatively few results for reflected processes or even reflected Brownian motions, especially in the context of oblique reflection and nonsmooth do-

mains which is relevant in applications. A convenient tool for the analysis of reflected Brownian motions is the so-called extended Skorokhod map (ESM), which maps an unconstrained trajectory to a version that is constrained to lie in a certain specified domain by applying a certain constraining force in the (possibly) oblique reflection vector field specified on the boundary. In [LR15] we first show that the analysis of pathwise differentiability of reflected Brownian motions can be reduced to the study of so-called directional derivatives of the associated ESM. For a special class of ESMs associated with the orthant and inwardly pointing directions of reflection, which arise in many applications, directional derivatives of the ESM were studied in previous work of Mandelbaum and Ramanan (2010). This class of ESMs are particular tractable because they exhibit a certain monotonicity property and admit a semi-explicit characterization. However, for more general ESMs that capture a broader range of applications, this monotonicity property does not hold and the approach of Mandelbaum and Ramanan can no longer be applied. In [LR15] we develop a completely new axiomatic framework for the characterization of directional derivatives of a much broader class of ESMs that are Lipschitz continuous. This work is a key step in future work that will study sensitivity analysis of functionals of RBMs, over both the finite and infinite time horizon.

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2.1 Preprints and publications

- CD13 Chowdhary, K. and Dupuis, P. Distinguishing and integrating aleatoric and epistemic variation in uncertainty quantification, *ESAIM: Mathematical Modelling and Numerical Analysis*, **47**, 2013, 635–662.
- BCD13 Budhiraja, A., Chen, J. and Dupuis, P. Large deviations for stochastic partial differential equations driven by a Poisson random measure, *Stochastic Processes and Their Applications*, **123**, 2013, 523–560.
- GRR14 Gantert, N., Ramanan, K. and Rembart, F. Large deviations for weighted sums of stretched exponential random variables, *Electronic Communications in Probability*, Volume 19, Article 41, 2014.
- ACD Atar, R., Chowdhary, K. and Dupuis, P. Robust bounds on risk-sensitive functionals via Rényi divergence, *SIAM/ASA J. Uncertainty Quantification*, **3**, 2015, 18–33.
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The AFOSR Program Officer currently assigned to the award

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Abstract

The project focused on the development, analysis, implementation, and application of efficient and high-order accurate methods for multi-scale and stochastic problems. Research focused on three topics:

- (1) High order weighted essentially non-oscillatory finite difference and finite volume schemes, discontinuous Galerkin finite element method, and related methods, for solving computational fluid dynamics (CFD) problems and other applications containing strong shock waves and complicated smooth region structures.
- (2) Development of higher order piecewise polynomial approximation for finite element methods.
- (3) The development of methods of simulation and analysis for the study of large scale stochastic systems of weakly interacting particles.

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Research Objectives

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Funding Summary by Cost Category (by FY, \$K)

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